UCRL-TR-235287

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Full-Process Computer Model of Magnetron Sputter, Part I: Test Existing State-of-Art Components

C. C. Walton, G. H. Gilmer, A. P. Wemhoff, L. A. Zepeda-Ruiz

October 4, 2007

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

UCRL-TR-235287

Title: Full-Process Computer Model of Magnetron Sputter, Part I: Test Existing State-of-Art Components

Project Overview

This work is part of a larger project to develop a modeling capability for magnetron sputter deposition. The process is divided into four steps: plasma transport, target sputter, neutral gas and sputtered atom transport, and film growth, shown schematically in Fig. 1. Each of these is simulated separately in this Part 1 of the project, which is jointly funded between CMLS and Engineering. The Engineering portion is the plasma modeling, in step 1.

The plasma modeling was performed using the Object-Oriented Particle-In-Cell code (OOPIC) from UC Berkeley [1]. Figure 2 shows the electron density in the simulated region, using magnetic field strength input from experiments by Bohlmark [2], where a scale of 1% is used. Figures 3 and 4 depict the magnetic field components that were generated using two-dimensional linear interpolation of Bohlmark's experimental data.

Project Goals

The goal of the overall modeling tool is to understand, and later predict, relationships between parameters of film deposition we can change (such as gas pressure, gun voltage, and target-substrate distance) and key properties of the results (such as film stress, density, and stoichiometry.) The simulation must use existing codes, either open-source or low-cost, not develop new codes. In part 1 (FY07) we identified and tested the best available code for each process step, then determined if it can cover the size and time scales we need in reasonable computation times. We also had to determine if the process steps are sufficiently decoupled that they can be treated separately, and identify any research-level issues preventing practical use of these codes. Part 2 will consider whether the codes can be (or need to be) made to talk to each other and integrated into a whole.

Relevance to LLNL Mission

LLNL has multiple projects depending on precision film deposition for critical goals. A prime example is control of film microstructure and stress in 180μm-thick sputtered Be metal shells for NIF targets. Others include stress control in large-area sputtered nanolaminate adaptive optics, and film stoichiometry in high-power capacitors.

FY07 Accomplishments and Results

In the plasma simulations, we developed an approach to a realistic plasma model, we eliminated computational heating, and we discovered the computational limitations of the plasma code. Figure 1 shows the largest obtainable domain size, 1% of real dimensions, which features a grid of 340×638 cells. We discovered that a 5% scale simulation using a grid of 1702×3192 cells crashes the code on a Windows platform, which calls for future work in implementing the research version of the code on high performance machines and developing a parallel electrostatic solver.

In the larger project we developed and partly validated models of the pressure and temperature distribution in the gas in front of the sputter gun. This model enabled us to calculate arrival angles and energies for sputtered Be atoms passing through the gas. These were then used as inputs for simulations of the growth of the Be films. These simulations already agree show columnar microstructure approaching a limiting grain size, with dome-shaped grains and a gap developing at the grain boundaries, all consistent with experiment and of key importance in understanding film density. An example of this qualitative agreement is shown in Fig. 5.

In the larger goal of testing all the separate codes for suitability, this project succeeded in identifying the plasma simulation as the most difficult of the four steps, showing us we must focus resources on it for the second year. We are negotiating a consulting contract with one of the authors of the plasma code, which will include parallel-processing capability since a single CPU seems to be insufficient for the system size we must simulate. All parts of this project are continuing in FY08 under programmatic and SI funding.

References

1. Verboncoeur, J. P., A. B. Langdon, and N. T. Gladd, "An object-oriented electromagnetic PIC code," *Comp. Phys. Comm.*, 87, pp. 199-211, 1995.
2. Bohlmark, J., U. Helmersson, M. VanZeeland, I. Axnas, J. Alami, and N. Brenning, "Measurement of the magnetic field discharge in a pulsed high current magnetron discharge," *Plasma Sources Sci. Technol.*, 13, pp. 654-661, 2004.

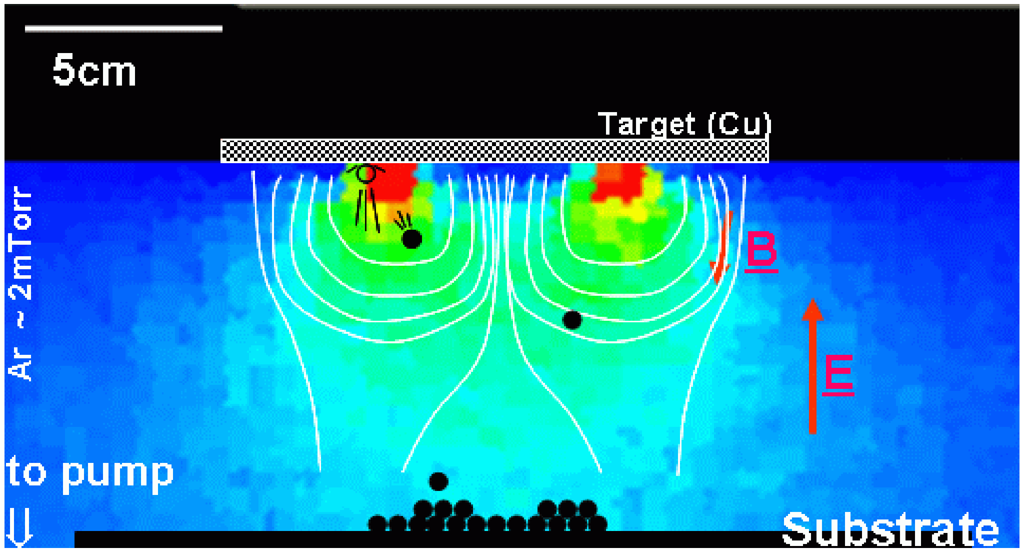

Fig. 1. Schematic of magnetron deposition system to be simulated in overall project. Engineering part consists of simulating charge species and interaction with **E** and **B** fields.

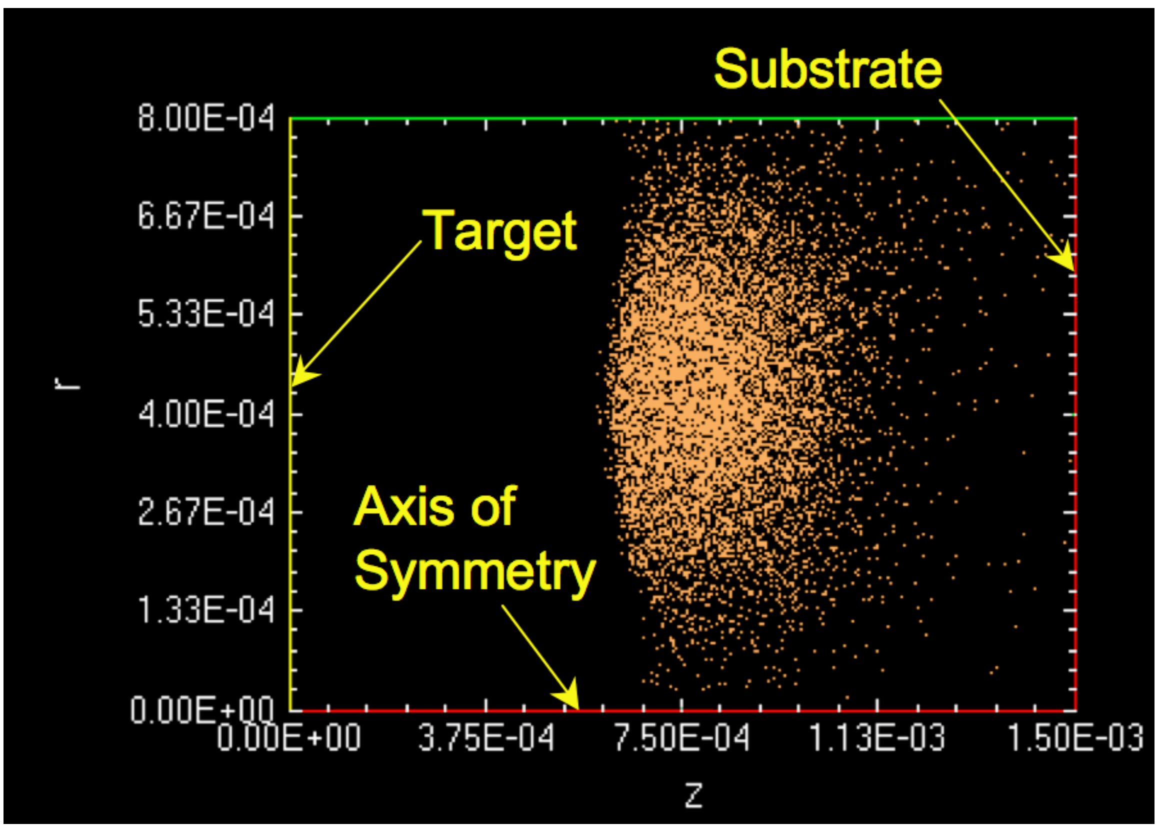

Figure 2. Test domain for plasma simulation, scaled 1%. Red points represent simulated clusters of electrons (Argon ions and neutral gas not shown).

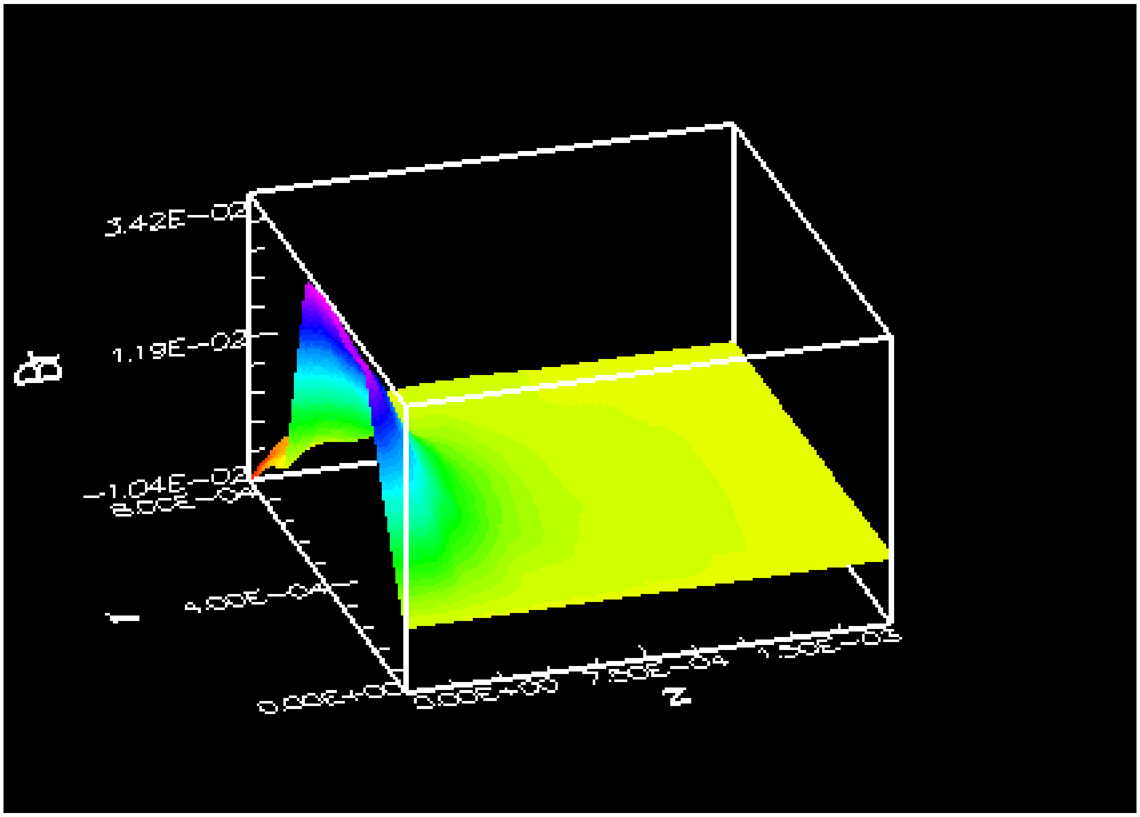

Figure 3. Radial magnetic field component used in plasma simulation.

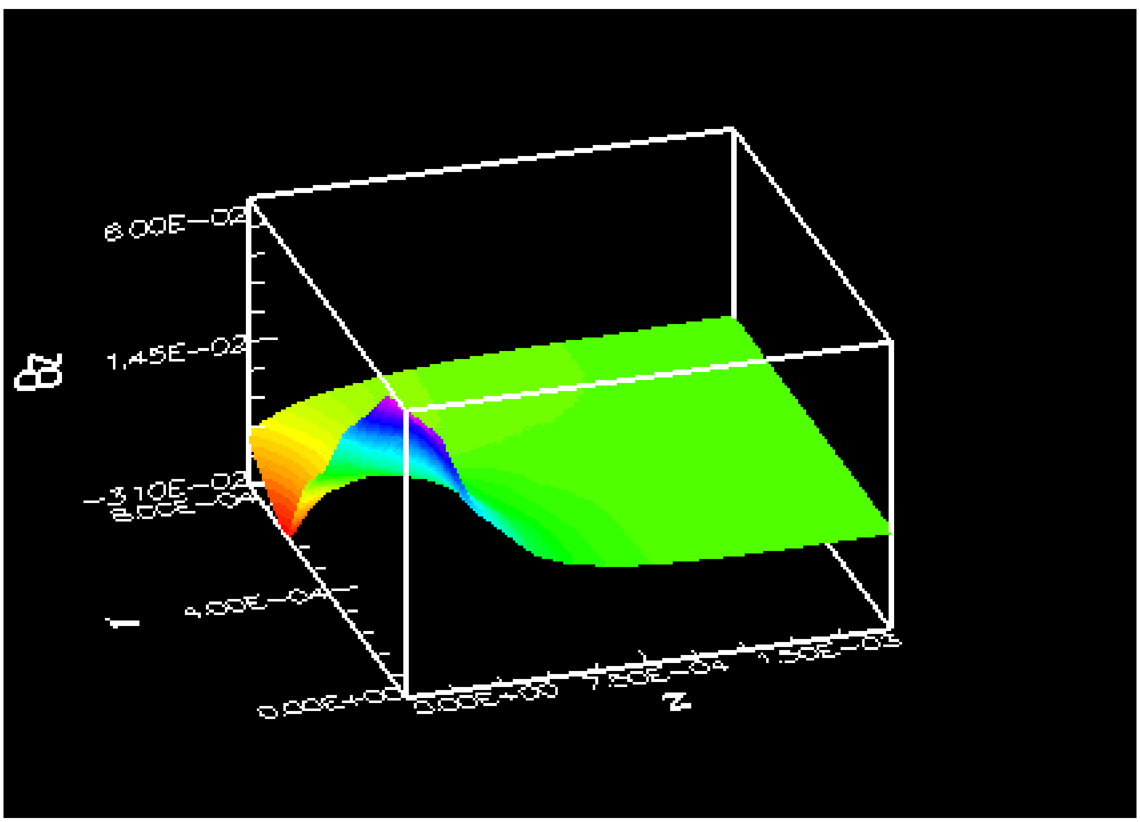

Figure 4. Axial magnetic field component used in plasma simulation.

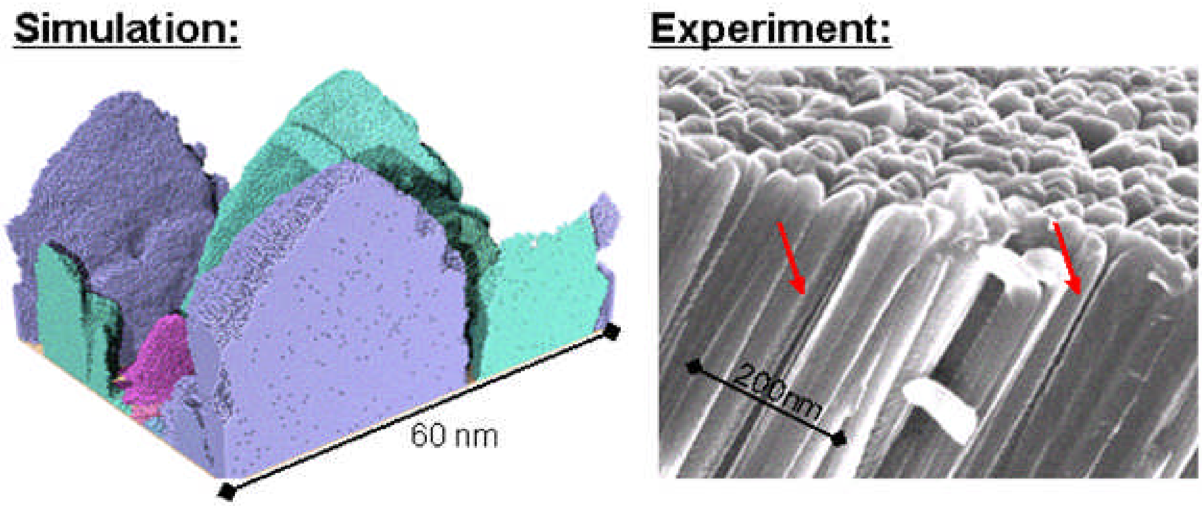

Figure 5. Simulated and experimental microstructure of sputtered Be films. Agreement of the columnar grains, reaching a steady-state width with dome-shaped tops and apparent gaps at the grain boundaries is our key qualitative result. Quantitative agreement remains as a future goal.